2-Methyl-2-propenyl p-tolyl sulphone

Inchi: InChI=1S/C11H14O2S/c1-9(2)8-14(12,13)11-6-4-10(3)5-7-11/h4-7H,1,8H2,2-3H3
InchiKey: KKSRFROTRSZRSD-UHFFFAOYSA-N
Formula: C11H14O2S
SMILES: C=C(C)CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 210.29
CAS: 16192-04-4

Physical Properties

Property code	Value	Unit	Source
chs	-6583.50 ± 1.20	kJ/mol	NIST Webbook
gf	-244.73	kJ/mol	Joback Method
hf	-241.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-348.00 ± 1.30	kJ/mol	NIST Webbook
hfus	26.69	kJ/mol	Joback Method
hsub	107.00 ± 3.00	kJ/mol	NIST Webbook
hvap	61.06	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.345		Crippen Method
mcvol	165.880	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
tb	527.08	K	Joback Method
tc	731.65	K	Joback Method
tf	275.51	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.55	J/mol×K	527.08	Joback Method
cpg	378.87	J/mol×K	561.18	Joback Method
cpg	393.33	J/mol×K	595.27	Joback Method
cpg	406.95	J/mol×K	629.37	Joback Method
cpg	419.75	J/mol×K	663.46	Joback Method
cpg	431.74	J/mol×K	697.56	Joback Method

cpg	442.94	J/mol×K	731.65	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16192044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume